NOVEL METHODS FOR ELECTROMAGNETIC SIMULATION AND
DESIGN

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Final Report

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14. ABSTRACT
The goal of this project was to develop a new generation of fast, robust, and accurate methods for solving the equations of electromagnetic scattering in realistic environments involving complex geometry. During the six year performance period (including a one-year no cost extension), we have made definitive progress in this direction. We have constructed new integral representations for scattering from perfect conductors and dielectrics that work across the frequency spectrum, are immune from low-frequency breakdown, and can be applied to surfaces of arbitrary genus. We have designed new quadrature methods (QBX for 'quadrature by expansion') which are high-order, efficient and easy to use on arbitrarily triangulated surfaces. The resulting discretized integral equations are compatible with fast multipoleaccelerated solvers and will form the basis for high fidelity modeling software that can handle complicated, electrically large objects in a manner that is sufficiently fast to allow design by simulation.

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Final Report

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Principal Investigator: Leslie Greengard

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Abstract: The goal of this project was to develop a new generation of fast, robust, and accurate methods for solving the equations of electromagnetic scattering in realistic environments involving complex geometry. During the six year performance period (including a one-year no cost extension), we have made definitive progress in this direction. We have constructed new integral representations for scattering from perfect conductors and dielectrics that work across the frequency spectrum, are immune from low-frequency breakdown, and can be applied to surfaces of arbitrary genus. We have designed new quadrature methods (QBX for "quadrature by expansion") which are high-order, efficient and easy to use on arbitrarily triangulated surfaces. The resulting discretized integral equations are compatible with fast multipole-accelerated solvers and will form the basis for high fidelity modeling software that can handle complicated, electrically large objects in a manner that is sufficiently fast to allow design by simulation.

We also developed new methods for scattering from cavities in a perfectly conducting half-space, for the simulation of layered and microstructured metamaterials, and for the analysis of time-domain integral equations. Finally, we have demonstrated the utility of our tools in predicting skin effects in MRI experiments on bulk metal samples.

Leslie Greengard, New York University

Scientific and Technical Activities and Findings

The ultimate goal of our research is to create a new generation of highly accurate methods for solving the equations of electromagnetic scattering in realistic environments involving complex geometry. To that end, we have developed, refined and implemented tools based on new mathematical representations that overcome many of the obstacles encountered by existing simulation techniques: ill-conditioning, low-frequency breakdown, and the inability to handle multi-connected domains in a robust fashion. We have also developing robust, high-order quadrature schemes for layer potentials defined on surfaces in three dimensions and direct solvers that will permit the efficient precomputation of the scattering responses of geometric substructures.

In our proposal, the targets were centered on:

- Modification of the FMM (fast multipole method) libraries to be able to handle the full Maxwell system

- Creation of a user interface that is compatible with piecewise smooth surface discretizations

- Development of high order quadrature methods for smooth surfaces

- Development of fast direct solvers

- Development of methods for inverting the surface Laplacian

- Development of integral equation methods for multiply connected domains.

- Implementation of fast algorithms on parallel computing platforms workstations

- Implementation of quadratures for corner and edge singularities

- Development of application layers for EMI and EMC (electromagnetic interference and compatibility).

- Initial development of fast direct solvers for the full Maxwell system and hybrid direct/iterative solvers

Background: After assembling a team in Year 1 with the necessary expertise, we constructed FMM libraries for the full Maxwell system, created a user interface compatible with both low and high order discretizations, and implemented the generalized Debye approach of [4]. The mathematical details of that approach were summarized in previous reports, and are omitted here.

Having completed the implementation, we made an important determination - namely that first order accurate quadrature schemes (which are widely used) would not be sufficiently accurate for reasonable mesh discretizations, so a major effort was initiated to design higher order quadratures that could be implemented efficiently. To provide some context, we note

that the classical formulation of the Maxwell equations (for scattering from a body Ω with boundary Γ) makes use of the vector and scalar potentials $\mathbf{A}$ and ϕ, induced by a surface current $\mathbf{J}$ [12, 16]:

$$\mathbf{E} = i\omega\mathbf{A} - \frac{1}{i\omega}\nabla\phi, \quad \mathbf{H} = \frac{1}{\mu}\nabla \times \mathbf{A}$$

with

$$\mathbf{A} = \int_\Gamma g(\mathbf{x} - \mathbf{y})\mathbf{J}(\mathbf{y})d\mathbf{y}, \quad \phi = \frac{1}{\epsilon}\int_\Gamma g(\mathbf{x} - \mathbf{y})\left(\nabla \cdot \mathbf{J}\right)(\mathbf{y})d\mathbf{y},$$

where

$$g(\mathbf{r}) = \frac{e^{ik|\mathbf{r}|}}{4\pi|\mathbf{r}|}.$$

Here, $\mathbf{E}$ and $\mathbf{H}$ are the electric and magnetic field, respectively, ϵ, μ are the permittivity and permeability, and ω is the frequency of interest. Using this formalism, the evaluation of the electromagnetic fields scattered by complicated objects in three dimensions requires the evaluation of the singular and weakly singular integrals that define $\mathbf{A}$ and ϕ above. The lack of efficient and high order rules for this purpose has been one of the fundamental obstacles to the development of robust design tools. During years 2-5 of the project, we developed a completely new approach to quadrature, which we refer to as QBX (quadrature by expansion) [13, 6]. Using only smooth rules, we are now able to evaluate local expansions of the fields induced by weakly singular, principal value and hypersingular integrals at a collection of off-surface points, from which we extract the one-sided limit of the layer potentials with surprising ease. A major effort over the past two years has been devoted to the development of hybrid QBX/FMM software so that layer potentials in complex geometry can be evaluated robustly, automatically and accurately with a simple user interface. We have completed a prototype code in two dimensions [17] and are now embarking on building the full three-dimensional version.

Selected Accomplishments:

• We completed a fast solver for inverse obstacle scattering and demonstrated what we believe are the most geometrically detailed, high frequency reconstructions to date (using simulated data [3]). The method is based on fast solvers coupled with recursive linearization.
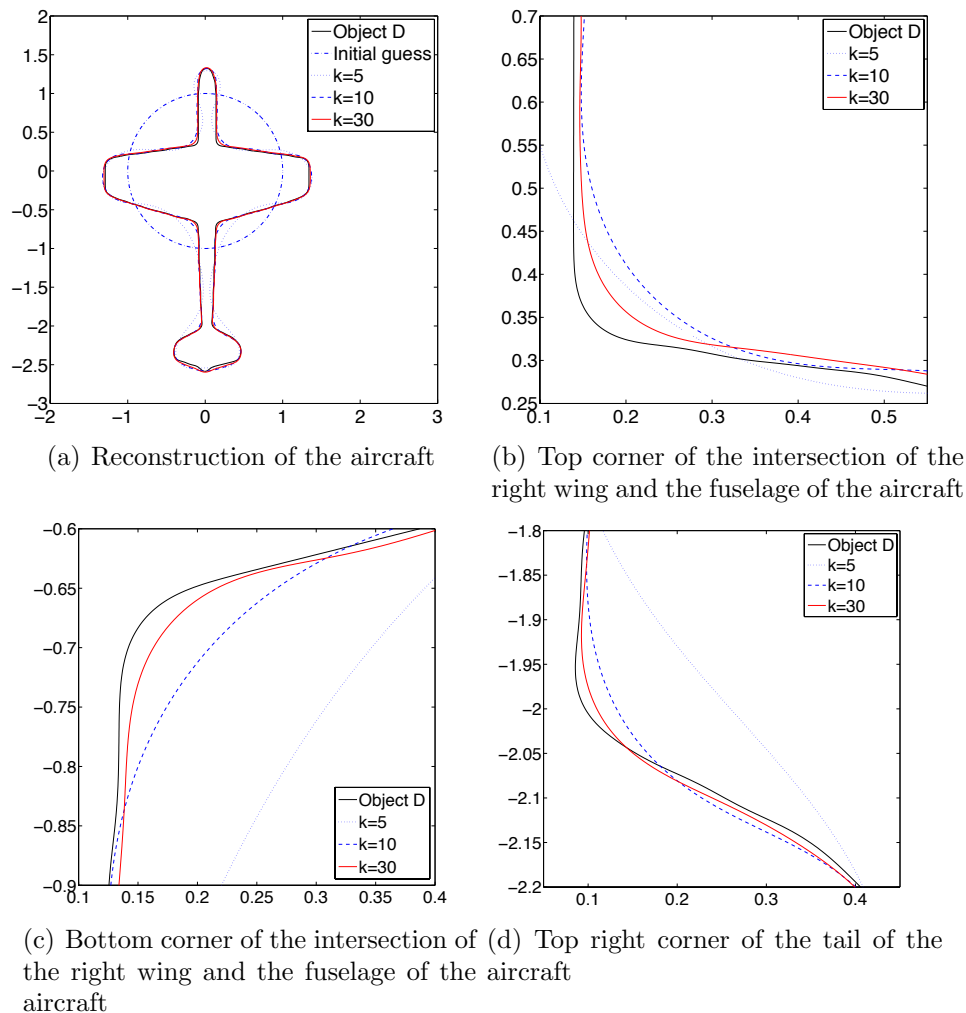

(a) Reconstruction of the aircraft

(b) Top corner of the intersection of the right wing and the fuselage of the aircraft

(c) Bottom corner of the intersection of the right wing and the fuselage of the aircraft

(d) Top right corner of the tail of the aircraft

Figure 1: Reconstruction of anaircraft-like object using recursive linearization and fast solvers (from [3]

• We began the development of a new approach to modeling scattering from layered media. Given a point source located in an unbounded half-space or an infinitely extended layer, Sommerfeld and others showed that Fourier analysis combined with contour integration provides a systematic and broadly effective approach, leading to what is generally referred to as the Sommerfeld integral representation. When either the source or target is at some distance from an infinite boundary, the number of degrees of freedom needed to resolve the scattering response is very modest. When both are near an interface, however,

the Sommerfeld integral involves a very large range of integration and its direct application becomes unwieldy. Historically, three schemes have been employed to overcome this difficulty: the method of images, contour deformation, and asymptotic methods of various kinds. None of these methods make use of classical layer potentials in physical space, despite their advantages in terms of adaptive resolution and high-order accuracy. The reason for this is simple: layer potentials are impractical in layered media or half-space geometries since they require the discretization of an infinite boundary. We developed a hybrid method which combines layer potentials (physical-space) on a finite portion of the interface together with a Sommerfeld-type (Fourier) correction. We have shown that our method is efficient and rapidly convergent for arbitrarily located sources and targets, and show that the scheme is particularly effective when solving scattering problems for objects which are close to the half-space boundary or even embedded across a layered media interface.

- We extended the frequency domain Lorenz-Mie-Debye formalism for the Maxwell equations to the time-domain. We showed that the problem of scattering from a perfectly conducting sphere can be reduced to the solution of two scalar wave equations one with Dirichlet boundary conditions and the other with Robin boundary conditions. An explicit, stable, and high-order numerical scheme was developed, based on our earlier treatment of the scalar case. This new representation may provide some insight into transient electromagnetic phenomena, and can also serve as a reference solution for general purpose time-domain software packages [8, 9].

- We extended the development of our formulation for electromagnetic scattering from perfect electric conductors to dielectrics. While our representation for the electric and magnetic fields is based on the standard vector and scalar potentials $\mathbf{A}, \phi$ in the Lorenz gauge, we established boundary conditions on the potentials themselves, rather than on the field quantities. This has permitted the development (for the first time) of a second kind Fredholm integral that avoids low frequency breakdown and is insensitive to the genus of the scatterer. The equations for the vector and scalar potentials are decoupled leading to what we call the "decoupled potential integral equation" [20].

- We developed a method for simulating acoustic or electromagnetic scattering in two dimensions from an infinite three-layer medium with thousands of wavelength-size dielectric particles embedded in the middle layer. Such geometries are typical of microstructured composite materials, and the evaluation of the scattered field requires a suitable fast solver for either a single configuration or for a sequence of configurations as part of a design or optimization process. We have developed an algorithm for problems of this type by combining the Sommerfeld integral representation, high order integral equation discretization, the fast multipole method and classical multiple scattering theory. [14].

- We developed new *randomized* methods for solving rank-deficient linear algebra problems [18]. This plays a role in our work on the magnetic field integral equation [5], but we believe it is of much broader utility.

- We applied our prototype full Maxwell solver to a problem in magnetic resonance imaing of bulk metals with experimental collaborators [7]. We showed that first principles RF field calculations can accurately predict NMR spectra.

- We developed a fast direct solver for the simulation of electromagnetic scattering from

an arbitrarily-shaped, large, empty cavity embedded in an infinite perfectly conducting half space. The governing Maxwell equations are reformulated as a well-conditioned second kind integral equation and the resulting linear system is solved in nearly linear time using a hierarchical matrix factorization technique. We have demonstrated the power of the technique with several numerical examples of complex cavity shapes over a wide range of frequencies [15].
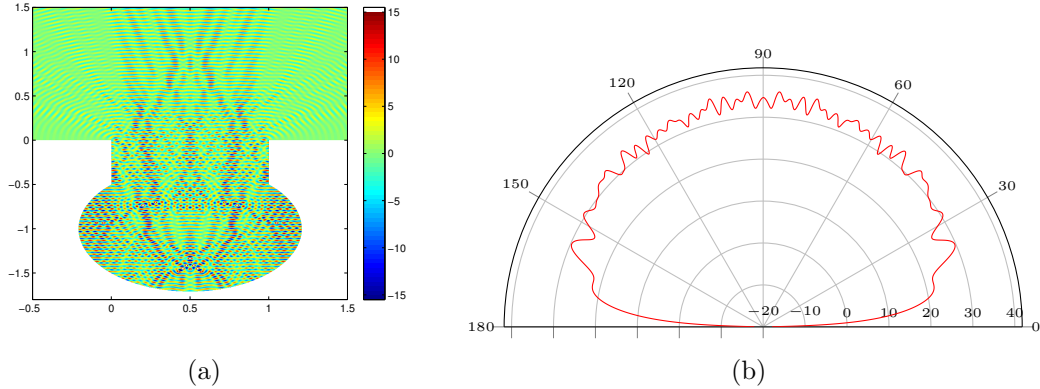

Figure 2: *(a) Real part of the scattered field for a pot shaped cavity with a normally incident plane wave at wavenumber k=160. (b) The backscatter RCS in dB for the pot shaped cavity at k=160*

• The interaction of acoustic or electromagnetic waves with structured, periodic materials is often complicated by the fact that the scattering geometry involves domains where multiple media meet at a single point (*triple-points*). For illustration, consider the geometry of a scattering problem shown in Fig. 3.

We developed a new integral equation method for the calculation of two-dimensional scattering from periodic structures involving triple-points [10]. The combination of a robust and high-order accurate integral representation and our previously developed fast direct solver [11] permits the efficient simulation of scattering from fixed structures at multiple angles of incidence (Fig. 4).
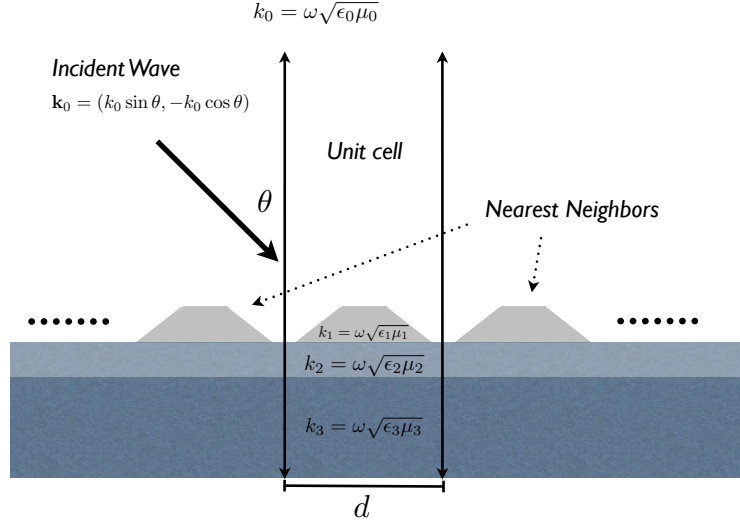
Figure 3: A periodic array of scatterers on the surface of a layered medium. The Helmholtz coefficient for the upper medium is k_0, that for the trapezoidal-shaped scatterers is k_1 and that of the two layers beneath are k_2 and k_3, respectively. We assume that the lowest interface (here between the k_2 and k_3 layers) is located at $y = 0$ and that the maximum height of the scatterers is at $y = y_0$. We also assume tha the unit cell is centered at $x = 0$. The bottom layer is assumed to be infinite in extent.
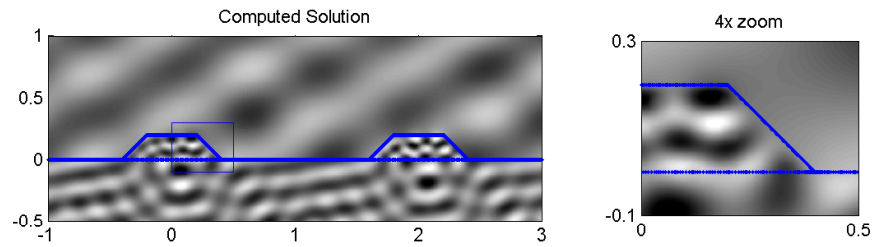

Figure 4: Real part of total field with plane incident wave.

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Budget

There were no significant changes to the original budget. We were staffed by a mixture of postdoctoral fellows, graduate students, visitors, and consultants.

Personnel

Senior research scientist **Zydrunas Gimbutas** accepted a position at NIST, where he is continuing to work in part on electromagnetics with a focus on magnetic resonance imaging applications. Postdoctoral fellows **Andreas Kloeckner** and **Josef Sifuentes** moved to faculty positions at the University of Illinois, Urbana-Champaign, and Texas A&M, respectively. Postdoctoral fellow **Michael O'Neil** began a faculty position at NYU in September, 2014. Postdoctoral fellow **Siva Ambikasaran** has taken a faculty position at the Indian Institute of Science, **Jun Lai** has taken a faculty position at Zhejiang University in China, and **Carlos Borges** is moving to the University of Texas, Austin for a second postdoctoral fellowship. NYU students **Manas Rachh** and **Travis Askham** took a Gibbs Instructorship at Yale and a postdoctoral fellowship at the University of Washington, respectively. Manas' dissertation focused on the QBX (quadrature) project and Travis worked on volume integral methods for variable coefficient media and problems with volume source terms.

At the University of Michigan, we supported one graduate student in Eric Michielssen's group, working on high frequency and time-domain scattering problems.

Our consultants have been **Charles Epstein** (U. Pennsylvania), **Eric Michielssen** (U. Michigan), **Shidong Jiang** (NJIT), and **Vladimir Rokhlin** (Yale U.). Prof. Epstein has worked on the analysis of the QBX quadrature scheme, integral equation theory, and the design of a method for smoothing edges and corners with user-controlled precision. Prof. Michielssen has concentrated on time-domain integral equation methods, and Prof. Rokhlin has concentrated on fast direct solvers and corner singularities. Prof. Jiang worked on time-domain methods.

Ways in which students and postdocs are contributing to the work

Students and postdocs were instrumental in virtually all aspects of this work. We developed a significantly different methodology compared with existing schemes, and made steady progress on multiple aspects of tool development.

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Publications

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Inventions or Patent Disclosures

None

Sabbatical or other professional development

Prof. Charles Epstein, Shidong Jiang, Eric Michielssen and Vladimir Rokhlin visited periodically to discuss work on the project and several group members have visited Yale University to work with Prof. Rokhlin. One graduate student (Manas Rachh) is now a Gibbs Assistant Professor at Yale, working with Prof. Rokhlin.

Awards and Honors

Leslie Greengard received the Wilbur Cross Medal from Yale University (2011), presented the John von Neumann Lecture at the SIAM Annual Meeting (2014), and was elected to the American Academy of Arts and Sciences (2016).

Accomplishments

- Implemented first solver for the Maxwell equations that is stable for all frequencies in simply or multiply connected geometries.

- Discovered previously unknown boundary conditions for electromagnetics in multiply connected domains that can be used to stabilize a variety of integral equation methods.

- Developed a simple and novel approach for constructing high order quadratures on complicated surfaces in three dimensions.

- Developed an efficient method for simulating layered, microstructured materials

- Developed the first integral representation for electromagnetic scattering from perfect conductors that is insensitive to the genus of the surface.

International Collaborations

Felipe Vico (Faculty, Universidad Politecnica de Valencia) visited our group on a regular basis. Prof. June-Yub Lee (Ehwa Womans University, Seoul, Korea) was a sabbatical visitor for an earlier project period and was partially supported by the NSSEFF grant. Motoki Kobayashi visited from Sony, Japan during the 2012-2013 academic year.

Interactions with DoD

Greengard served on the Air Force Studies Board, and has been in occasional contact with the electromagnetics (CREATE) project at WPAFB (Drs. John D'Angelo, Ryan Chilton) and with Dr. Ruth Pachter a Senior Scientist the Air Force Research Laboratory, Materials and Manufacturing Directorate at WPAFB.

Group members (including the PI) attended the annual AFOSR Electromagnetics Contractor's Meetings. Greengard was invited to present lectures at the 2013, 2014, and 2015 meetings.

1.

1. Report Type

Final Report

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Abstract

The goal of this project was to develop a new generation of fast, robust, and accurate methods for solving the equations of electromagnetic scattering in realistic environments involving complex geometry. During the six year performance period (including a one-year no cost extension), we have made definitive progress in this direction. We have constructed new integral representations for scattering from perfect conductors and dielectrics that work across the frequency spectrum, are immune from low-frequency breakdown, and can be applied to surfaces of arbitrary genus. We have designed new quadrature methods (QBX for "quadrature by expansion") which are high-order, efficient and easy to use on arbitrarily triangulated surfaces. The resulting discretized integral equations are compatible with fast multipole-accelerated solvers and will form the basis for high fidelity modeling software that can handle complicated, electrically large objects in a manner that is sufficiently fast to allow design by simulation.

We completed a fast solver for inverse obstacle scattering and demonstrated what we believe are the most geometrically detailed, high frequency reconstructions to date (using simulated data. The method is based on fast solvers coupled with recursive linearization.

We extended the frequency domain Lorenz-Mie-Debye formalism for the Maxwell equations to the time-

domain. We showed that the problem of scattering from a perfectly conducting sphere can be reduced to the solution of two scalar wave equations — one with Dirichlet boundary conditions and the other with Robin boundary conditions. An explicit, stable, and high-order numerical scheme was developed, based on our earlier treatment of the scalar case. This new representation may provide some insight into transient electromagnetic phenomena, and can also serve as a reference solution for general purpose time-domain software packages.

We developed a method for simulating acoustic or electromagnetic scattering in two dimensions from an infinite three-layer medium with thousands of wavelength-size dielectric particles embedded in the middle layer. Such geometries are typical of microstructured composite materials, and the evaluation of the scattered field requires a suitable fast solver for either a single configuration or for a sequence of configurations as part of a design or optimization process. We have developed an algorithm for problems of this type by combining the Sommerfeld integral representation, high order integral equation discretization, the fast multipole method and classical multiple scattering theory.

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Equipment/Facilities			
Supplies			
Total			

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